

**A COURSE SYLLABUS – DOCTORAL SCHOOL**  
REGARDING THE QUALIFICATION CYCLE FROM 2024/2025 TO 2028/2029

<b>GENERAL INFORMATION ABOUT COURSE</b>				
Course title	<b>DOCTORAL DISSERTATION</b>			
Name of the unit running the course	Doctoral School at University of Rzeszów			
Type of course ( <i>obligatory, optional</i> )	obligatory subject			
Year and semester of studies	year I -IV, semester: I - VIII			
Discipline	Physical science			
Language of Course	Polish/English language			
Name of Course coordinator	Dr. Rafał Hakalla, prof. UR			
Name of Course lecturer	Dr. Rafał Hakalla, prof. UR			
Prerequisites	Range of knowledge, skills and competencies derived from the graduate program in physics. Knowledge of the English language at a level that allows the use of foreign-language sources of scientific information, preparation of publications and presentation of scientific achievements at specialized conferences.			
<b>BRIEF DESCRIPTION OF COURSE</b> (100-200 words)				
The dissertation workshop focuses on supporting the next stages of the research procedure, the implementation of which is crucial for the preparation of the dissertation. The content of the course focuses on preparing sources of spectra of the selected molecule, obtaining high-quality spectra of this molecule by modern methods of high resolution spectroscopy, conducting extended spectral analysis of the strongly and extensively perturbed ro-vibronic states of the speck, in order to work out its physical and chemical properties, which can be used in space programs and astrophysical and astronomical projects.				
<b>COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES</b>				
Learning outcome	The description of the learning outcome defined for the course	Relation to the degree programme outcomes (symbol)	Learning Format (Lectures, classes,...)	Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...)
<b>Knowledge (no.)</b>	knows and understands, has knowledge			
<b>P8S_WG1</b>	To the extent that it is possible to revise existing paradigms - a worldwide body of work, including theoretical foundations and general issues and selected specific issues - specific to high-resolution molecular spectroscopy;	<b>P8S_WG</b>	conversation	Report (publication)
<b>P8S_WG2</b>	On the main development trends of high-resolution spectroscopy;	<b>P8S_WG</b>	conversation	Report (publication)
<b>P8S_WG3</b>	Knows, understands and can apply professional terms used in high resolution molecular spectroscopy, in native and foreign language;	<b>P8S_WG</b>	conversation	Report (publication)
<b>P8S_WG4</b>	issues in the methodology of conducting scientific research	<b>P8S_WG</b>	conversation	Report (publication)

	of high resolution spectroscopy; principles of planning and implementation of scientific research, using interdisciplinary research techniques and tools;			
<b>Skills (no.)</b>	can			
<b>P8S_UW<sub>1</sub></b>	based on his knowledge of various fields of science, is able to identify and solve problems of high-resolution molecular spectroscopy, define the purpose, formulate the hypothesis and the object of scientific research, improve spectroscopic research techniques, methods and tools, and make conclusions based on the results of scientific research;	<b>P8S_UW</b>	conversation	Report (publication)
<b>P8S_UW<sub>2</sub></b>	select and use scientific literature to diagnose and solve research problems and innovative activities in their research work, and apply the appropriate workshop to create new elements of scientific achievements;	<b>P8S_UW</b>	conversation	Report (publication)
<b>P8S_UW<sub>3</sub></b>	independently acquire knowledge, expand analytical skills, and stimulate critical sensitivity to recognize dilemmas in conducting scientific research and fulfilling the role of a university teacher;	<b>P8S_UW</b>	conversation	Report (publication)
<b>Social competence (no.)</b>	is ready to			
<b>P8S_KK<sub>1</sub></b>	critically evaluate the achievements within the framework of high-resolution molecular spectroscopy, and critically assess the contribution of the results of one's own research activities to the development of the discipline.	<b>P8S_KK</b>	conversation	Report (publication)

#### LEARNING FORMAT – NUMBER OF HOURS

Semester (no.)	Lectures	Seminars	Lab classes	Internships	others	ECTS
<b>I - VIII</b>	-	<b>8 x 5 hrs. - 40 hrs.</b>	<b>8 x 25 hrs. - 200 hrs.</b>	-	-	<b>24</b>

#### METHODS OF INSTRUCTION

- CONVERSATIONS IN THE TRADITIONAL FORM;
- PROJECTS;
- DISCUSSION;
- INTERPRETATION OF SOURCE TEXTS;
- PERFORMING EXPERIMENTS AND EXPERIMENTS;

## COURSE CONTENT

### **Doctoral dissertation**

#### Semester I

Topic: Development of a customized methodology for the measurement and spectroscopic analysis of a selected molecule taking into account appropriate research techniques.

Topic : Designing and commissioning a source of spectra of a selected diatomic molecule.

Topic : Obtaining the ro-vibronic spectrum of a molecule in the selected measurement range.

#### Semester II

Topic: Identifying the spectrum associated with the first vibrational level of a key electronic state.

Topic: Selection of theoretical analytical methods appropriate for high resolution spectroscopy.

#### Semester III

Topic: Performing deperturbation analysis for the first vibrational level of the key electronic state.

Topic: Obtaining and presenting results and formulating conclusions and predictions.

Topic: Writing a scientific article presenting the obtained results.

#### Semester IV

Topic: Identifying the spectrum associated with the next vibrational level of the key electronic state.

Topic: Perform deperturbation analysis for the next vibrational level of the key electronic state.

Topic: Obtaining and presenting the results and making conclusions and predictions.

Topic: Writing a scientific article presenting the obtained results.

#### Semester V

Topic: Carrying out deperturbation analysis for the next two vibrational levels of the key electronic state.

Topic: Obtaining and presenting the results and making conclusions and predictions.

Topic: Writing two scientific papers presenting the obtained results.

#### Semester VI

Topic : Performing a global deperturbation analysis involving all analyzed vibrational levels of the key electronic state.

Topic : Writing a scientific article presenting the obtained results.

#### Semester VII and VIII

Topic : Writing a PhD dissertation.

## COURSE ASSESSMENT CRITERIA

The evaluation is based on the continuous work of the doctoral student in each semester and academic year in terms of: implementation of research, expansion of knowledge, study of literature, involvement and progress in the preparation of the dissertation. Possible semester grades are: 2.0, 3.0, 3.5, 4.0, 4.5, 5.0.

Sample percentage requirements for the grading scale:

To obtain a passing grade, a conversion factor is used for the corresponding percentage of points obtained:

- up to 50% - insufficient, (the doctoral student does not make progress in scientific research, does not expand his knowledge, does not study the readings, does not participate in substantive discussion, does not fulfill his scientific duties);

- 51% - 60% - sufficient, (the doctoral student makes negligible progress in scientific research, expands knowledge, studies primary literature, the discussion held is limited to a narrow range of substantive knowledge, fulfills basic scientific duties);

- 61% - 70% - sufficient plus, (the doctoral student makes progress in scientific research, expands knowledge, studies basic literature, substantively participates in the discussion, fulfills scientific duties);

- 71% - 80% - good, (doctoral student makes significant progress in scientific research, expands knowledge, studies primary and secondary literature, substantively participates in discussion, fulfills all scientific duties);

- 81% - 90% - good plus, (the doctoral student makes significant progress in scientific research, systematically expands knowledge, studies basic and complementary literature, substantively participates in discussion, fulfills all scientific duties);

- 91% - 100% - very good (the doctoral student makes significant progress in scientific research, systematically expands knowledge, studies basic, complementary and beyond the obligatory literature, substantively participates in discussion, fulfills all scientific duties);

TOTAL PhD STUDENT WORKLOAD REQUIRED TO ACHIEVE THE INTENDED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS	
Activity	Number of hours
Scheduled course contact hours	8 x 30 hrs - 240 hrs.
Other contact hours involving the teacher (consultation hours, examinations)	10
Non-contact hours – student's own work (preparation for classes or examinations, project, etc.)	470
<b>Total number of hours</b>	720
<b>Total number of ECTS credits</b>	24

### INSTRUCTIONAL MATERIALS

Compulsory literature:	<ol style="list-style-type: none"> <li>1. P. W. Atkins, <i>Physical Chemistry</i>, 11th edition, Oxford University Press, 2018.</li> <li>2. <i>Handbook of High-Resolution Spectroscopy</i>, Vol. 1-3, ed. by M. Quack and F. Merkt, Wiley, 2011.</li> <li>3. P. F. Bernath, <i>Spectra of Atoms and Molecules</i>, 4th Edition, Oxford University Press, 2020.</li> <li>4. G. Herzberg, <i>Molecular Spectra and Molecular Structure, vol. I: Spectra of Diatomic Molecules</i>, (2<sup>nd</sup> edition), Krieger Publishing Company, Malabar, Florida, 1989.</li> <li>5. J. T. Hougen, <i>The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules</i>, National Institute of Standards and Technology (NIST), Monograph 115, 1970.</li> <li>6. H. Lefebvre-Brion, R.W. Field, <i>The Spectra and Dynamics of Diatomic Molecules</i>, Elsevier, 2004.</li> <li>7. J. M. Brown and A. Carrington, <i>Rotational Spectroscopy of Diatomic Molecules</i>, Cambridge University Press, 2003.</li> <li>8. N. Colin, N. Banwell and E. M. McCash, <i>Fundamentals of Molecular Spectroscopy</i>, 4th Edition, McGraw-Hill, 2021.</li> <li>9. H. Haken and H. C. Wolf, <i>Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory</i>, 2nd Edition, Springer, 2004.</li> <li>10. H. Haken and H. C. Wolf, <i>The Physics of Atoms and Quanta</i>, 7th Edition, Springer, 2005.</li> </ol>
Complementary literature:	<ol style="list-style-type: none"> <li>1. J. Sadlej „Spektroskopia molekularna”, WNT, 2002</li> <li>2. W. Kołos, J. Sadlej „Atom i cząsteczka”, WNT, 1998</li> <li>3. W. Kołos „Chemia kwantowa”, PWN, 1978</li> <li>4. P. Kowalczyk „Fizyka cząsteczek. Energie i widma”, PWN, 1999.</li> <li>5. A. Gołębiewski „Elementy mechaniki i chemii kwantowej”, PWN, 1982.</li> <li>6. Z. Leś „Wstęp do spektroskopii atomowej”, PWN 2014.</li> </ol>

\*(1 ECTS CREDIT CORRESPONDS TO 25 - 30 HOURS OF THE TOTAL WORKLOAD OF A DOCTORAL STUDENT, NEEDED TO ACHIEVE THE ESTABLISHED EFFECTS).

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Date and signature of the Course lecturer

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Approved by the Head of the Department or an authorised person